

# Worst-case multi-objective error estimation and adaptivity

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## Abstract

This paper introduces a new computational methodology for determining a-posteriori multi-objective error estimates for finite-element approximations, and for constructing corresponding (quasi-)optimal adaptive refinements of finite-element spaces. As opposed to the classical goal-oriented approaches, which consider only a single objective functional, the presented methodology applies to general closed convex subsets of the dual space and constructs a worst-case error estimate of the finite-element approximation error. This worst-case multi-objective error estimate conforms to a dual-weighted residual, in which the dual solution is associated with an approximate supporting functional of the objective set at the approximation error. We regard both standard approximation errors and data-incompatibility errors associated with incompatibility of boundary data with the trace of the finite-element space. Numerical experiments are presented to demonstrate the efficacy of applying the proposed worst-case multi-objective error in adaptive refinement procedures.

*Keywords:* a-posterior error estimation, worst-case multi-objective error estimation, adaptive finite-element methods,

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## 1. Introduction

Goal-oriented *a-posteriori* error-estimation and adaptivity has emerged over the past years as an effective methodology to solve measurement problems in computational science and engineering. As opposed to the classical norm-oriented adaptive methods that originated from the seminal work of Babuška and Rheinboldt [1, 2], which aim to construct finite-element approximations that are optimal in an appropriate norm, goal-oriented adaptive methods seek to construct finite-element approximations that yield optimal approximations of a particular functional of the solution. Goal-oriented methods date back to the pioneering work of Becker and Rannacher [4, 5], Oden and Prudhomme [30, 28] and Giles, Süli, Houston and Hartmann [14, 20, 16, 17]. It is noteworthy, however, that the use of dual solutions in a-posteriori error estimates, which forms

the basis of goal-oriented error estimation, had already been pursued before by Johnson, Eriksson and Hansbo [10, 21, 22]. Goal-oriented adaptivity has been successfully applied to a wide variety of problems including compressible and incompressible flow problems [17, 31, 32], elasticity and plasticity [37, 33, 34], variational inequalities [38], fluid-structure interaction [45, 13, 36, 6], free-boundary problems [46, 47], phase-field models [42, 44], and kinetic equations [19]. This overview is in fact far from exhaustive, and many more applications and contributions can be found in the literature. It is notable, however, that despite the success of goal-oriented methods in many applications, convergence and optimality theory is still rudimentary; see [26, 12].

In addition to goal-oriented adaptivity of the mesh width ( $h$ ) or local order ( $p$ ) of finite-element approximation spaces, goal-oriented approaches have also been considered in the context of model adaptivity. In these approaches, the error indicator is applied to systematically decide between a simple coarse model and a complex sophisticated model, in such a manner that the sophisticated model is only applied in regions of the domain that contribute most significantly to the objective functional under consideration. For examples of goal-oriented model adaptivity, we refer to [29] for application of goal-oriented model adaptivity to heterogeneous materials, to [3] for goal-oriented atomistic/continuum adaptivity in solid materials, and to [43] for goal-oriented adaptivity between a boundary-integral formulation of the Stokes equations and a PDE formulation of the Navier-Stokes equations.

The premise in goal-oriented strategies is that interest is restricted to a single functional output, rather than all details of the solution of the system under consideration. Although there are indeed many applications in which interest is restricted to a single scalar output of a system, there are in fact many more in which the object of interest is not so narrowly defined. There are for instance many applications in which multiple scalar outputs are of interest, e.g. the aerodynamic drag, lift and torques that are exerted by a flow on an immersed object [15]. Another example is furnished by the many cases in which one is concerned with the solution in a particular region of the problem domain. This scenario also covers boundary-coupled multiphysics problems, e.g. fluid-structure interaction [45], in which two subsystems interact via a mutual interface and only one of the subsystems is of importance, and free-boundary problems [46, 47], in which interest extends to the geometry of the domain only and not to the solution of the underlying partial differential equation, or vice versa. A similar situation arises for volumetrically-coupled multiphysics problems, e.g. electro-thermo-mechanical problems [24], if significance is assigned to one field only. Another pertinent class of problems that are incompatible with the premise of goal-oriented strategies, pertains to applications in which one is interested in the flux functional on a part of the boundary that is subjected to essential boundary conditions or, reciprocally, the trace of the solution on a part of the boundary that is furnished with natural boundary conditions. In all of the aforementioned cases, interest does not extend to all details of the solution, but it is also not restricted to a single quantity. Instead, the objective set in these cases corresponds to a proper non-singleton subset of the dual space, and

not to an individual element of the dual space as in goal-oriented approaches.

The purpose of this paper is to introduce a new computational methodology for determining a-posteriori *multi-objective* error estimates for finite-element approximations, and for constructing corresponding (quasi-)optimal adaptive refinements of finite-element spaces. Such multi-objective error estimation and adaptivity has only received scant consideration so far; see [11, 15]. As opposed to the aforementioned approaches, our methodology applies to generic possibly infinite-dimensional closed convex subsets of the dual space. The presented methodology relies on the construction of a worst-case error estimate, viz. the supremum of the error over the objective set. This worst-case error corresponds to the value of the supporting function of the objective set at the finite-element approximation error. We then construct an approximate supporting functional of the objective set at the approximation error, and determine an approximate dual solution for this supporting functional to form an error estimate in dual-weighted-residual form [4]. The corresponding error estimate represents a *worst-case multi-objective error estimate* for the finite-element approximation on the objective set. In this work, we regard both standard approximation errors and data-incompatibility errors associated with incompatibility of boundary data with the trace of the finite-element space.

The presented worst-case multi-objective error estimate is based on a technique for estimating linear functionals of solutions of equations with unbounded closed linear operators set in Hilbert spaces [48]. This technique applies to general linear operators with non-trivial null-spaces and possibly non-closed ranges, and it is based on an extension of Young–Fenchel duality to closed unbounded linear operators [50, 48]. It is noteworthy that this technique for estimating a linear functional of a solution of an operator equation, which we consider in this paper in the context of worst-case multi-objective error estimation, yields a natural generalization of adaptive-state-estimation or so-called data-assimilation procedures (such as online sequential filters [40, 51, 39] or offline variational approaches [18]) to a wide class of linear and nonlinear partial differential equations, enabling incorporation of a-posteriori knowledge (for instance, sensor readings) into the error estimate rendering it less conservative [51, 49].

The remainder of this paper is organized as follows. Section 2 presents a model problem that serves as a concrete setting for the worst-case multi-objective error-estimation procedure. In this section we also review standard goal-oriented error estimation. Section 3 introduces worst-case multi-objective error estimation in an abstract Hilbert-space setting. We consider both standard finite-element-approximation errors and errors engendered by data incompatibility. In Section 4, we conduct numerical experiments to illustrate the properties of the worst-case multi-objective error-estimation procedure, and we consider its application in an adaptive-refinement procedure. Section 5 presents concluding remarks.

## 2. Model problem and preliminaries

To provide a concrete background for the presented worst-case multi-objective error-estimation and adaptivity processes, and to elucidate aspects related to data incompatibility and boundary conditions, we consider the standard Dirichlet–Poisson problem. A general setting is presented in Section 3.

### 2.1. Problem statement

Consider a bounded open subset  $\Omega \subset \mathbb{R}^d$  ( $d = 2, 3$ ) with boundary  $\partial\Omega$ . We assume throughout that  $\Omega$  is a Lipschitz domain, with boundary  $\Gamma := \partial\Omega$ . We consider the standard Dirichlet–Poisson problem:

$$-\Delta u = f \quad \text{in } \Omega \quad (1a)$$

$$u = g \quad \text{on } \Gamma \quad (1b)$$

where  $f : \Omega \rightarrow \mathbb{R}$  and  $g : \Gamma \rightarrow \mathbb{R}$  are exogenous functions.

To accommodate the weak formulation of (1), let  $H^1(\Omega)$  denote the Sobolev space of square-integrable functions with square-integrable (in Lebesgue sense) weak derivatives, equipped with the standard scalar product, norm and semi-norm, here denoted by  $(\cdot, \cdot)_{H^1(\Omega)}$ ,  $\|\cdot\|_{H^1(\Omega)}$  and  $|\cdot|_{H^1(\Omega)}$ , respectively. We denote by  $\gamma : H^1(\Omega) \rightarrow L^2(\Gamma)$  the trace operator, defined via the continuous extension of the operator that restricts continuous functions on  $\Omega$  to the boundary  $\Gamma$ . The trace space  $H^{1/2}(\Gamma) := \gamma H^1(\Omega)$  corresponds to a proper subspace of  $L^2(\Gamma)$ . We denote by  $H_0^1(\Omega)$  the kernel of  $\gamma$ , viz. the subclass of functions in  $H^1(\Omega)$  that vanish on  $\Gamma$  in the trace sense. In addition, we denote by  $\ell_{(\cdot)} : H^{1/2}(\Gamma) \rightarrow H^1(\Omega)$  a suitable right-inverse of  $\gamma$ . Such a right inverse is generally called a lift operator. Lift operators are non-unique. A particular example is the (harmonic) Moore–Penrose lift associated with the  $H^1$ -semi norm:

$$g \mapsto \arg \min \{ |v|_{H^1(\Omega)} : v \in H^1(\Omega), \gamma v = g \} \quad (2)$$

The boundary value problem (1) can now be condensed into the weak formulation: given  $f \in L^2(\Omega)$  and  $g \in H^{1/2}(\Gamma)$ , find

$$u \in \ell_g + H_0^1(\Omega) : \quad a(u, v) = b(v) \quad \forall v \in H_0^1(\Omega) \quad (3)$$

where the bilinear form  $a : [H^1(\Omega) \times H^1(\Omega)]^*$  and linear form  $b \in [H^1(\Omega)]^*$  are defined by:

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v, \quad b(v) = \int_{\Omega} f v \quad (4)$$

with  $(\cdot)^*$  the topological dual of  $(\cdot)$ . Weak problem (3) with non-homogeneous boundary data  $g$  and lift  $\ell_g$  admits a reinterpretation as:

$$u_0 \in H_0^1(\Omega) : \quad a(u_0, v) = b(v) - a(\ell_g, v) \quad \forall v \in H_0^1(\Omega) \quad (5)$$

followed by the additive composition  $u = \ell_g + u_0$ .

## 2.2. Galerkin finite-element approximations

Consider a strictly decreasing sequence of mesh parameters  $\mathcal{H} = (h_i)_{i \in \mathbb{Z}_{\geq 0}}$  with only accumulation point zero, and a corresponding sequence of asymptotically dense nested (finite-element) approximation spaces  $V^{h_0} \subset V^{h_1} \subset V^{h_2} \subset \dots \subset H^1(\Omega)$ . With each  $h \in \mathcal{H}$  we associate a discrete lift operator  $\ell_{(\cdot)}^h : H^{1/2}(\Gamma) \rightarrow V^h$  such that  $\gamma(\ell_g^h)$  is close to  $g$  in some appropriate sense. Denoting by  $V_0^h$  the intersection of  $V^h$  and  $H_0^1(\Omega)$ , composed of approximation functions in  $V^h$  that vanish on the boundary, we associate with each  $h \in \mathcal{H}$  the Galerkin approximation problem:

$$u^h \in \ell_g^h + V_0^h : \quad a(u^h, v^h) = b(v^h) \quad \forall v^h \in V_0^h \quad (6)$$

Defining the *residual* operator  $r : H^1(\Omega) \rightarrow [H^1(\Omega)]^*$  according to

$$\text{for all } (u, v) \in H^1(\Omega) \times H^1(\Omega) : \quad \langle r(u), v \rangle = b(v) - a(u, v) \quad (7)$$

we note for later reference that the residual corresponding to the Galerkin approximation  $u^h$  in (6) is orthogonal with respect to the test functions  $V_0^h$ , i.e.,  $\langle r(u^h), v^h \rangle$  vanishes for all  $v^h \in V_0^h$ .

## 2.3. Goal-oriented error estimation

Consider a functional  $j \in [H^1(\Omega)]^*$  and suppose that interest is restricted to  $j(u)$  with  $u$  according to (3), rather than to the all details of the solution to (3). A problem of this type is called a *measurement problem* and  $j$  is generally referred as a *goal functional*, *target functional* or *objective functional*. By virtue of the Riesz representation theorem, the functional  $j(\cdot)$  can generally be written in the form:

$$j(\cdot) = a(\cdot, \vartheta) \quad (8)$$

with  $\vartheta \in H^1(\Omega)$ . The trace of  $\vartheta$  is associated with a weak (so-called *variationally consistent*) formulation of the flux  $\partial_n u$  [41, 25]. Indeed, if  $u$  satisfies (1), then the following integration by parts identity holds for all  $\vartheta \in H^1(\partial\Omega)$ :

$$\int_{\partial\Omega} (\gamma\vartheta) \partial_n u = \int_{\Omega} \nabla \vartheta \cdot \nabla u + \int_{\Omega} \vartheta \Delta u = a(u, \vartheta) - b(\vartheta) =: \langle \gamma\vartheta, \partial_n u \rangle \quad (9)$$

The functional  $\langle \gamma\vartheta, \partial_n(\cdot) \rangle$  is affine and consists of a linear part,  $a(\cdot, \vartheta)$  and a translation,  $b(\vartheta)$ . The translation depends exclusively on data of the problem, and is therefore in principle explicitly computable. Only the linear part  $a(u, \vartheta)$  of  $\langle \gamma\vartheta, \partial_n u \rangle$  depends on the solution.

We associate with (3) and the goal functional  $j$  the following *dual problem*:

$$z \in H_0^1(\Omega) : \quad a(v, z) = j(v) \quad \forall v \in H_0^1(\Omega) \quad (10)$$

In this context, problem (3) is referred to as the *primal problem*. It is to be noted that the function  $z$  corresponds to the Riesz representation of  $j$  in  $H_0^1(\Omega)$  with inner product  $a(\cdot, \cdot)$ . In view of the representation of  $j$  in (8), the dual problem (10) can alternatively be conceived of as a projection from  $H^1(\Omega)$

into  $H_0^1(\Omega)$ . We will denote this projection by  $\pi_0(\cdot)$ . For any  $\vartheta \in H^1(\Omega)$ , the complement  $\vartheta - \pi_0\vartheta$  corresponds to the weakly harmonic lift of the trace of  $\vartheta$ . To corroborate this assertion, we note that by (8) and (10) it holds that  $a(v, \vartheta - \pi_0\vartheta) = 0$  for all  $v \in H_0^1(\Omega)$ , which implies that  $\vartheta - \pi_0\vartheta$  is weakly harmonic. Evidently, it moreover holds that  $\gamma(\vartheta - \pi_0\vartheta) = \gamma\vartheta$ .

Consider the Galerkin approximation  $u^h = u_0^h + \ell_g^h \in V^h$  to  $u$  according to (6). The dual solution enables us to express the error in the objective functional,  $j(u) - j(u^h)$ , without direct reference to the error in the approximation. The error representation follows from the following sequence of identities:

$$\begin{aligned} j(u) - j(u^h) &= j(\ell_g - \ell_g^h) + j(u_0 - u_0^h) \\ &= j(\ell_g - \ell_g^h) + a(u_0 - u_0^h, z) \\ &= j(\ell_g - \ell_g^h) - a(\ell_g - \ell_g^h, z) + b(z) - a(u^h, z) \\ &= a(\ell_g - \ell_g^h, \vartheta - \pi_0\vartheta) + \langle r(u^h), \pi_0\vartheta - v^h \rangle \end{aligned} \tag{11}$$

for all  $v^h \in V_0^h$ . The first identity follows from the partitions  $u = u_0 + \ell_g$  and  $u^h = u_0^h + \ell_g^h$ . The second identity holds on account of  $u_0 - u_0^h \in H_0^1(\Omega)$  and the dual problem (10). The third identity follows from the primal problem in the form (5) and a partition of zero. The fourth identity follows from (7) and (8) and a rearrangement of terms, in combination with the property  $\langle r(u^h), v^h \rangle = 0$  for all  $v^h \in V_0^h$  of the Galerkin approximation. It is to be noted that the error-representation formula, viz., the ultimate expression in (11), depends on the approximation  $u^h$  only via the corresponding residual.

The first term in the error representation can be conceived of as the error induced by a discrepancy in the data of the weak formulation (3) and its Galerkin finite-element approximation (6). Typically, this discrepancy results from an incompatibility of the boundary data, viz.  $g \notin \gamma V^h$ . The second term represents the standard *Dual-Weighted Residual (DWR)* contribution to the error in the objective functional [4]. In particular, the error representation conveys that the contribution of the boundary-data error,  $\ell_g - \ell_g^h$ , to the error in the objective functional vanishes if the representation function of the objective functional,  $\vartheta$ , is compactly supported in  $\Omega$ , i.e. if  $\vartheta \in H_0^1(\Omega)$ . It then holds that the projection  $\pi_0\vartheta$  coincides with  $\vartheta$ . Therefore, the DWR term separately provides an error representation if the boundary conditions are compatible or if the trace of the representation function of the objective functional vanishes.

*Remark.* Two alternative error-representation formulas can be derived, in addition to the final expression in (11). To this end, let us consider the Galerkin approximation of the dual problem (10) in the finite-element approximation space  $V^h$ :

$$z^h \in V_0^h : \quad a(v^h, z^h) = j(v^h) \quad \forall v^h \in V_0^h \tag{12}$$

Denoting by  $\rho : H^1(\Omega) \rightarrow [H^1(\Omega)]^*$  the *dual residual*,

$$\text{for all } (u, v) \in H^1(\Omega) \times H^1(\Omega) : \quad \langle \rho(v), u \rangle = j(u) - a(u, v) \tag{13}$$

we infer that the residual of the Galerkin approximation  $z^h$  to the dual solution according to (12) satisfies the orthogonality relation  $\langle \rho(z^h), v^h \rangle = 0$  for all  $v^h \in V^h$ . Therefore,

$$\begin{aligned} j(u) - j(u^h) &= j(\ell_g - \ell_g^h) + j(u_0 - u_0^h) \\ &= a(\ell_g - \ell_g^h, \vartheta) + j(u_0) - a(u_0, z^h) + (a(u_0, z^h) - a(u_0^h, z^h)) \quad (14) \\ &= a(\ell_g - \ell_g^h, \vartheta - z^h) + \langle \rho(z^h), u_0 - u_0^h \rangle \end{aligned}$$

for all  $v^h \in V_0^h$ . Hence, the error in the goal functional,  $j(u) - j(u^h)$ , can alternatively be expressed as the sum of a data-incompatibility contribution and the duality pairing of the dual residual associated with the Galerkin approximation of the dual solution,  $\rho(z^h)$ , and an interpolation error in the homogeneous part of the primal solution in  $V_0^h$ , i.e.,  $u_0 - v^h$  for some  $v^h \in V_0^h$ . It is to be noted, however, that the first term in the ultimate expression in (14) generally vanishes only if  $\ell_g - \ell_g^h = 0$  and not if  $\vartheta \in H_0^1(\Omega)$ , as opposed to the data-incompatibility contribution in (11).

In the absence of data-incompatibility errors, we can also infer the following *symmetric error representation* from (11) and (14):

$$j(u) - j(u^h) = \frac{1}{2} \langle r(u^h), z - w^h \rangle + \frac{1}{2} \langle \rho(z^h), u - v^h \rangle \quad (15)$$

for all  $v^h, w^h \in V_0^h$ . For nonlinear problems, i.e., for semi-linear forms  $a(\cdot, \cdot)$  and nonlinear goal functionals  $j(\cdot)$ , the error representations generally deviate from the exact error on account of linearization errors. The primal and dual error estimates exhibit quadratic remainders, i.e., the error estimates deviate from  $j(u) - j(u^h)$  by  $O(\|u - u^h\|_{H^1(\Omega)}^2)$  as  $\|u - u^h\|_{H^1(\Omega)} \rightarrow 0$ . The symmetric error representation has the advantage that it exhibits a third order remainder; see [5].

The worst-case multi-objective error-estimation process proposed in this paper and the corresponding adaptive procedure are based on the error representation (11). ■

### 3. Worst-case multi-objective error estimation

In many applications, interest does not extend to all details of a solution to a boundary-value problem, but it is also not restricted to a single objective functional. Instead, one can envisage situations in which all functionals in a proper subclass of the dual space are of concern. Accordingly, to assess the accuracy of an approximation to the solution, an estimate of the associated error in all functionals in the considered subclass is required. In this section we propose a methodology for constructing such a *multi-objective error estimate*, based on the worst-case error.

#### 3.1. Worst-case multi-objective error estimation without data incompatibility

We formulate the worst-case multi-objective error estimate in an abstract setting encompassing the model problem presented in Section 2. For simplicity, we first restrict ourselves to error estimates without data-incompatibility

contributions (cf. Section 2.3), so that the DWR error-representation formula for objective functionals applies directly. The extension to error estimates with data incompatibility is treated in Section 3.2.

Let  $H$  denote a Hilbert space with inner product  $(\cdot, \cdot)_H$  and induced norm  $\|\cdot\|_H$ . The dual space  $H^*$  of  $H$  consists of all continuous linear functionals on  $H$ , equipped with the dual norm  $\|\cdot\|_{H^*} = \sup\{\langle \cdot, v \rangle : v \in H, \|v\|_H = 1\}$ . We consider a continuous and coercive bilinear form  $a \in [H \times H]^*$ , a continuous linear form  $b \in H^*$ , and the problem:

$$u \in H : \quad a(u, v) = b(v) \quad \forall v \in H \quad (16)$$

The Lax-Milgram Lemma (see, for instance, [7, Thm 2.7.7]) asserts that under the aforementioned hypotheses on  $a$  and  $b$ , problem (16) is well posed and that the solution  $u$  to (16) satisfies the a-priori estimate  $\|u\|_H \leq C\|b\|_{H^*}$  for some positive constant  $C > 0$ . Denoting by  $H^h \subset H$  a proper subspace of  $H$ , the Galerkin approximation of (16) in  $H^h$  writes:

$$u^h \in H^h : \quad a(u^h, v^h) = b(v^h) \quad \forall v^h \in H^h \quad (17)$$

Assuming that interest is restricted to a closed and convex class of objective functionals  $\mathcal{O} \subset H^*$ , it is appropriate to assess the accuracy of the approximation  $u^h$  according to (17) not with reference to its deviation from the solution  $u$  in the  $\|\cdot\|_H$ -norm, but by the deviation between  $j(u)$  and  $j(u^h)$  for all  $j \in \mathcal{O}$ . Concentrating on the largest deviation, the *support function*  $s(\mathcal{O}, u - u^h)$  of  $\mathcal{O}$  at  $u - u^h$  therefore constitutes an appropriate error measure. The support function  $s(\mathcal{O}, \cdot) : H \rightarrow \mathbb{R}$  of a closed convex set  $\mathcal{O} \subset H^*$  is defined as:

$$s(\mathcal{O}, v) = \sup \{ \langle j, v \rangle : j \in \mathcal{O} \} \quad (18)$$

The supremum in (18) is in fact attained by a functional in  $\mathcal{O}$  by virtue of  $\mathcal{O} \subset H^*$  being closed. A maximizing functional  $j_s \in H^*$  such that  $j(v) \leq j_s(v)$  for all  $j \in \mathcal{O}$  is referred to as a *supporting functional* of  $\mathcal{O}$  at  $v$ .

*Remark.* An equivalent characterization of the worst-case multi-objective error  $s(\mathcal{O}, u - u^h)$  is provided by

$$\sup \{ \langle r(u^h), z \rangle : z \in H \text{ such that } a(v, z) = j(v) \text{ for all } v \in H, j \in \mathcal{O} \}$$

with  $r : H \rightarrow H^*$ ,  $\langle r(u), \cdot \rangle := b(\cdot) - a(u, \cdot)$  the residual functional associated with (16) at  $u$ ; cf. (7) and (10)–(11). Young–Fenchel duality implies that the supremum in (19) coincides with the support function of  $\mathcal{O}$  at  $x \in H$ , that is

$$s(\mathcal{O}, x) = \sup \{ \langle r(u^h), z \rangle : z \in H \text{ such that } a(v, z) = j(v) \text{ for all } v \in H, j \in \mathcal{O} \} \quad (19)$$

provided

$$x \in H : \quad a(x, v) = \langle r(u^h), v \rangle \quad \forall v \in H \quad (20)$$

Noting that  $\langle r(u^h), v \rangle = b(v) - a(u^h, v) = a(u - u^h, v)$ , we infer that  $x = u - u^h$  and, indeed, the supremum in (19) coincides with  $s(\mathcal{O}, u - u^h)$ . ■



Based on a supporting functional  $j_s \in H^*$  of the objective set  $\mathcal{O}$  at the error  $u - u^h$ , an upper bound to the worst-case multi-objective error can be constructed which depends on the approximation  $u^h$  only via the corresponding residual,  $r(u^h)$ . The worst-case multi-objective error bound assumes the conventional DWR form; cf. (10) and (19). Denoting by  $z \in H$  the dual solution associated with the considered supporting functional of  $\mathcal{O}$  at  $u - u^h$ ,

$$z \in H : \quad a(w, z) = j_s(w) \quad \forall w \in H. \quad (21)$$

the following sequence of inequalities holds:

$$\sup_{j \in \mathcal{O}} |j(u) - j(u^h)| \leq j_s(u - u^h) = a(u - u^h, z) = b(z) - a(u^h, z) = \langle r(u^h), z \rangle \quad (22)$$

The upper bound in (22) is sharp if  $j_s \in \mathcal{O}$ . If the approximation  $u^h$  corresponds to the Galerkin approximation in (17), then  $\langle r(u^h), v^h \rangle$  vanishes for all  $v^h \in H^h$  and, accordingly, any interpolant of  $z$  in  $H^h$  can be subtracted in the ultimate expression in (22).

Application of the above theory in actual computations requires the construction of (a suitable approximation of) the support function of the objective set  $\mathcal{O}$  at the error  $u - u^h$ . In addition, if the worst-case multi-objective error estimate serves to direct an adaptivity procedure based on a DWR formulation, then the supporting functional of  $\mathcal{O}$  at  $u - u^h$  is also required. Below we consider support functions and supporting functionals for three specific classes of  $\mathcal{O}$ . Exemplifications in the context of the model problem of Section 2 are provided in Section 4.

*Example 1.* In our first example we consider the case of  $\mathcal{O}$  represented by a convex combination of a finite set of functionals, i.e. given  $\{j_1, \dots, j_n\} \subset H^*$ ,

$$\mathcal{O} = \left\{ j \in H^* : j = \sum_{i=1}^n \alpha_i j_i, \sum_{i=1}^n \alpha_i = 1, \alpha_i \in \mathbb{R}_{\geq 0} \right\} \quad (23)$$

For any error  $u - u^h \in H$ , it then follows that there exists an index  $\tilde{i} \in [1, \dots, n]$  such that  $j_{\tilde{i}}$  is a supporting functional of  $\mathcal{O}$  at  $u - u^h$ :

$$\begin{aligned} s(\mathcal{O}, u - u^h) &= \sup \{ \langle j, u - u^h \rangle : j \in \mathcal{O} \} = \sup \left\{ \sum_{i=1}^n \alpha_i \langle j_i, u - u^h \rangle : \sum_{i=1}^n \alpha_i = 1, \alpha_i \in \mathbb{R}_{\geq 0} \right\} \\ &= \max \{ \langle j_i, u - u^h \rangle : i \in [1, \dots, n] \} = \langle j_{\tilde{i}}, u - u^h \rangle \end{aligned} \quad (24)$$

Note that the index  $\tilde{i}$  generally depends on  $u - u^h$ . The worst-case multi-objective error  $s(\mathcal{O}, u - u^h)$  can thus be expressed as  $s(\mathcal{O}, u - u^h) = \langle j_{\tilde{i}}, x \rangle$  with  $x$  according to (20).

*Example 2.* Our second example concerns the case that  $\mathcal{O}$  coincides with the unit ball in  $H^*$ :

$$\mathcal{O} = \{ j \in H^* : \|j\|_{H^*} \leq 1 \}. \quad (25)$$

For any error  $u - u^h$ , a supporting functional of  $\mathcal{O}$  according to (25) at  $u - u^h$  is then provided by  $(u - u^h, \cdot)_H / \|u - u^h\|_H$ . Indeed, denoting by  $\phi : H^* \rightarrow H$  the canonical isometry between  $H^*$  and  $H$ , it holds for any  $u - u^h \in H$  that

$$\begin{aligned} s(\mathcal{O}, u - u^h) &= \sup \{ \langle j, u - u^h \rangle : j \in H^*, \|j\|_{H^*} \leq 1 \} = \sup \{ (\phi(j), u - u^h)_H : j \in H^*, \|j\|_{H^*} \leq 1 \} \\ &= \sup \{ (v, u - u^h)_H : v \in H, \|v\|_H \leq 1 \} = (u - u^h, u - u^h)_H / \|u - u^h\|_H \end{aligned} \quad (26)$$

Hence,  $s(\mathcal{O}, u - u^h) = (u - u^h, x) / \|u - u^h\|_H$  with  $x$  according to (20).

*Example 3.* As a preliminary to describe the third example, we consider a Hilbert space  $V \supseteq H$  with inner product  $(\cdot, \cdot)_V$  and norm  $\|\cdot\|_V$ , such that the embedding  $\iota : H \rightarrow V$  is continuous. Let  $B : V \rightarrow V$  denote a continuous linear operator. The third example pertains to the objective set

$$\mathcal{O} = \left\{ j \in H^* : j(\cdot) = (\iota(\cdot), Bv)_V, v \in V, \|v\|_V \leq 1 \right\} \quad (27)$$

That is,  $\mathcal{O}$  corresponds to the  $V$ -inner product with the image of the unit ball in  $V$  under the linear operator  $B$ . For any  $u - u^h \in H$ , the following sequence of identities holds:

$$\begin{aligned} s(\mathcal{O}, u - u^h) &= \sup \{ \langle j, u - u^h \rangle : j \in \mathcal{O} \} \\ &= \sup \{ (\iota(u - u^h), Bv)_V : v \in V, \|v\|_V \leq 1 \} \\ &= \sup \{ (B^* \iota(u - u^h), v)_V : v \in V, \|v\|_V \leq 1 \} \\ &= (B^* \iota(u - u^h), B^* \iota(u - u^h))_V / \|B^* \iota(u - u^h)\|_V \end{aligned} \quad (28)$$

with  $B^* : V \rightarrow V$  the adjoint operator of  $B$  in  $V$ . From (28) we infer that

$$s(\mathcal{O}, u - u^h) = \frac{(B^* \iota(u - u^h), B^* \iota(x))_V}{\|B^* \iota(u - u^h)\|_V} \quad (29)$$

with  $x$  according to (20). A particular instance of this third example in the context of the model problem of Section 2.1 is addressed in Section 4.

### 3.2. Worst-case multi-objective error estimation with data incompatibility

To provide a generic setting for worst-case multi-objective error estimation with data incompatibility, we consider a Hilbert space  $H$  and a proper subspace  $H_0 \subset H$ . Let  $a \in [H \times H]^*$  and  $b \in H^*$  denote continuous bilinear and linear forms, respectively. In addition, we assume that  $a$  is coercive on  $H_0$ , i.e.  $a(u, u) \geq \underline{c}_a \|u\|_H^2$  for some constant  $\underline{c}_a > 0$  for all  $u \in H_0$ . Given an element  $\ell \in H$  and an objective functional  $j \in H^*$ , we consider the measurement problem of determining  $j(u)$  with  $u = \ell + u_0$  and  $u_0 \in H_0$  according to:

$$u_0 \in H_0 : \quad a(u_0, v) = b(v) - a(\ell, v) \quad \forall v \in H_0 \quad (30)$$

Suppose that  $\ell$  is not explicitly available, but instead we only have access to an approximation  $\ell^h \in H$  with data error  $\ell - \ell^h$ . Given a subspace  $H_0^h \subset H_0$ , we consider the approximation  $u^h = \ell^h + u_0^h$ ,

$$u_0^h \in H_0^h : \quad a(u_0^h, v^h) = b(v^h) - a(\ell^h, v^h) \quad \forall v^h \in H_0^h \quad (31)$$

and, in particular, the corresponding approximate measurement,  $j(u^h)$ . Without loss of generality, we assume that the objective functional can be written in the general form  $j(\cdot) = a(\cdot, \vartheta)$  for some  $\vartheta \in H$ ; cf. (8). A derivation analogous to (11) then conveys that

$$j(u) - j(u^h) = a(u - u^h, \vartheta) = a(\ell - \ell^h, \vartheta - \pi_0 \vartheta) + \langle r(u^h), \pi_0 \vartheta - v^h \rangle \quad (32)$$

for all  $v^h \in H_0^h$  and with  $\pi_0 \vartheta \in H_0$  the projection of  $\vartheta$  onto  $H_0$  according to the dual problem:

$$\pi_0 \vartheta \in H_0 : \quad a(v, \pi_0 \vartheta) = a(v, \vartheta) \quad \forall v \in H_0 \quad (33)$$

Equation (32) imparts that the data error contributes to the measurement error only via  $\vartheta - \pi_0 \vartheta$ . We can therefore restrict our analysis of data-incompatibility errors to objective sets  $\mathcal{O} \subseteq \{a(\cdot, \vartheta) : \vartheta \in H_0^\perp\}$  with  $H_0^\perp := (1 - \pi_0)H$ .

We assume that the objective set  $\mathcal{O}$  is generated by the image of the map  $\lambda \mapsto a(\cdot, L(\lambda))$ , where  $L : T \rightarrow H_0^\perp$  corresponds to a linear operator from a Hilbert space  $T$  into  $H_0^\perp$ . The inner product and norm associated with  $T$  are denoted by  $(\cdot, \cdot)_T$  and  $\|\cdot\|_T$ , respectively. In particular, we consider the objective set:

$$\mathcal{O} = \{j \in H^\star : j(\cdot) = a(\cdot, L(\lambda)), \lambda \in T, \|\lambda\|_T \leq 1\} \quad (34)$$

By virtue of the continuity of  $L : T \rightarrow H_0^\perp$  and of  $a \in [H \times H]^\star$ , it holds that  $\hat{j}(\cdot) := a(u - u^h, L(\cdot)) \in T^\star$ . Denoting by  $\phi : T^\star \rightarrow T$  the canonical isometry between  $T^\star$  and  $T$ , the worst-case multi-objective data-error can be expressed as:

$$\sup \{\hat{j}(\lambda) : \lambda \in T, \|\lambda\|_T \leq 1\} = \sup \{(\phi(\hat{j}), \lambda)_T : \lambda \in T, \|\lambda\|_T \leq 1\} \quad (35)$$

The supremum in (35) is attained at  $\lambda = \phi(\hat{j})/\|\phi(\hat{j})\|_T$ , yielding the value  $\|\phi(\hat{j})\|_T$ .

Instead of the error representation corresponding to the ultimate expression in (32), we have used the error representation according to the second expression in (32) to formulate the worst-case multi-objective error representation in (35). The reason for this is that in practice, the lift  $\ell$  which appears in the ultimate expression in (32) will not be explicitly available, and needs to be replaced by a suitable approximation. It is then more convenient and not more restrictive to apply the second expression in (32) with the exact solution  $u$  replaced by a suitable approximation. Based on various orthogonality properties, many distinct and equivalent forms of the error representation can be derived; see Sections 4.3 and 4.4.

## 4. Numerical Experiments

We consider four different numerical experiments to elucidate the main properties of the worst-case multi-objective error estimator and its application in adaptive-refinement procedures. The first test case addresses the properties of the error estimate without data incompatibility with various polynomial orders of the finite-element approximation, for a problem with regular primal and dual solutions. The second test case illustrates the application of the error estimate in the absence of data incompatibility to guide an adaptive-refinement process, for a problem in which the primal and dual solutions exhibit restricted regularity on account of a corner singularity. The third and final test cases are concerned with error estimation and adaptivity for a problem with nearly singular incompatible boundary data and heterogeneous coefficients.

### 4.1. Worst-case multi-objective error estimation without data incompatibility

The first test case concerns the Dirichlet–Poisson problem (1) on a bi-unit square  $\Omega = (-1, 1)^2$ . The data  $f$  and  $g$  are selected such that

$$u_{\text{osc}}(x, y) = \sin(6\pi x) \sin(6\pi y) \quad (36)$$

solves (1). Note that the solution  $u_{\text{osc}}$  is smooth (of class  $C^\infty$ ) and displays moderate oscillatory behavior, and that the trace of  $u_{\text{osc}}$  on  $\partial\Omega$  vanishes and, hence, the corresponding Dirichlet data  $g$  is homogeneous. The considered Dirichlet–Poisson problem can be condensed into the weak formulation:

$$u \in H_0^1(\Omega) : \quad a(u, v) = b(v) \quad \forall v \in H_0^1(\Omega) \quad (37)$$

with the bilinear form  $a(\cdot, \cdot)$  corresponding to (4) and the linear form  $b(\cdot) = a(u_{\text{osc}}, \cdot)$ , with  $u_{\text{osc}}$  according to (36). By virtue of the homogeneity of the Dirichlet data, the finite-element approximations are devoid of data-incompatibility errors. Moreover, the smoothness of  $u_{\text{osc}}$  ensures that finite-element approximations on uniform meshes display optimal convergence behavior, in particular,  $\|u^h - u_{\text{osc}}\|_{H^k(\Omega)} \leq Ch^{p+1-k}$  ( $k \in \{0, 1\}$ ) for some constant  $C > 0$  independent of the mesh width  $h$ , with  $p$  the polynomial degree of the finite-element space.

We set  $H := H_0^1(\Omega)$ ,  $V := L^2(\Omega)$  and consider the objective set

$$\mathcal{O} = \{j \in [H^1(\Omega)]^* : j(\cdot) = (\cdot, \chi_\omega v)_{L^2(\Omega)}, \|v\|_{L^2(\Omega)} \leq 1\} \quad (38)$$

with  $\chi_\omega$  the indicator function of the set  $\omega = (-3/4, -1/4)^2$ . The support function of  $\mathcal{O}$  at  $u - u^h$  characterizes the  $L^2$ -norm of the error in  $u^h$  in the subset  $\omega$ . Indeed, it holds that  $\chi_\omega^* = \chi_\omega$  and, hence,

$$\begin{aligned} \sup \{(u - u^h, \chi_\omega v)_{L^2(\Omega)} : \|v\|_{L^2(\Omega)} \leq 1\} &= \sup \{(\chi_\omega(u - u^h), v)_{L^2(\Omega)} : \|v\|_{L^2(\Omega)} \leq 1\} \\ &= \|\chi_\omega(u - u^h)\|_{L^2(\Omega)} \end{aligned} \quad (39)$$

The considered Dirichlet–Poisson problem with objective set  $\mathcal{O}$  according to (38) conforms to the third example treated in Section 3. By analogy to (29), we infer that

$$j_s(\cdot) = \frac{(\chi_\omega(u - u^h), \cdot)_{L^2(\Omega)}}{\|u - u^h\|_{L^2(\Omega)}}$$

is a supporting functional of  $\mathcal{O}$  at  $u - u^h$ . Therefore, if  $u^h$  is determined from the Galerkin approximation (6), then  $s(\mathcal{O}, u - u^h) = \langle r(u^h), z - v^h \rangle$  for any  $v^h \in V_0^h$ , with  $z \in H_0^1(\Omega)$  according to the dual problem

$$z \in H_0^1(\Omega) : \quad a(v, z) = \frac{(\chi_\omega(u - u^h), v)_{L^2(\Omega)}}{\|u - u^h\|_{L^2(\Omega)}} \quad \forall v \in H_0^1(\Omega) \quad (40)$$

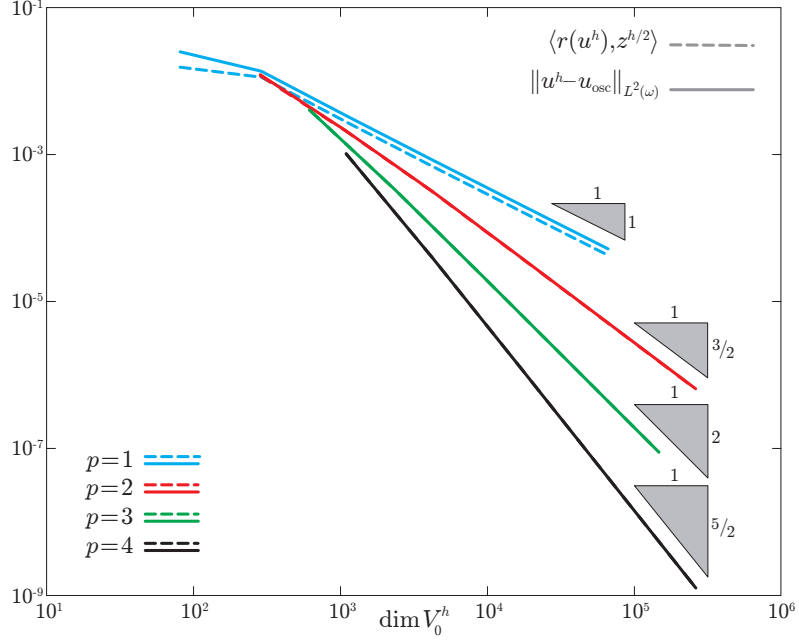
In practice, the exact solution  $u$  is unavailable, and an estimate of the error  $u - u^h$  is required to construct an approximate supporting functional. In the numerical computations, we apply finite-element approximation spaces based on rectangular elements, and we opt to approximate the error in (40) by  $u^{h/2} - u^h$ , where  $u^{h/2}$  is an approximation obtained from a Galerkin approximation in a finite-element space  $V_0^{h/2}$  in which each element is uniformly divided into 4 elements; see Figure 2. The refined finite-element space  $V_0^{h/2}$  moreover serves to construct an approximation to the dual solution in (40). In summary, considering an approximation  $u^h \in V_0^h$  and a refined approximation  $u^{h/2} \in V_0^{h/2}$ , the worst-case multi-objective error estimate pertaining to  $u^h$  is  $\langle r(u^h), z^{h/2} \rangle$  with  $z^{h/2}$  according to

$$z^{h/2} \in V_0^{h/2} : \quad a(v^{h/2}, z^{h/2}) = \frac{(\chi_\omega(u^{h/2} - u^h), v^{h/2})_{L^2(\Omega)}}{\|\chi_\omega(u^{h/2} - u^h)\|_{L^2(\Omega)}} \quad \forall v^{h/2} \in V_0^{h/2} \quad (41)$$

Figure 1 plots the worst-case multi-objective error estimate,  $\langle r(u^h), z^{h/2} \rangle$ , versus the dimension of the finite-element approximation space,  $\dim V_0^h$ , for finite-element approximations with polynomial degrees  $p \in \{1, 2, 3, 4\}$  on uniform meshes with mesh width  $h = 2^{-2}, 2^{-3}, \dots$ . To verify the accuracy of the worst-case multi-objective error estimate, the figure also plots the exact error  $\|u^h - u_{\text{osc}}\|_{L^2(\omega)}$ . It is noteworthy that both the worst-case multi-objective error estimate and the exact error exhibit optimal convergence rates proportional to  $(\dim V_0^h)^{-(p+1)/2}$ . The deviation between the worst-case multi-objective error estimate and the exact error is generally small. For  $p = 1$ , the error estimate underestimates the error by approximately 25% on the coarsest mesh and by approximately 10% on all finer meshes. For  $p \in \{2, 3, 4\}$ , the deviation between the error estimate and the exact error is not discernible.

#### 4.2. Worst-case multi-objective error estimation and adaptivity without data incompatibility

In the second test case we examine the application of the worst-case multi-objective error estimate to direct an adaptive-refinement procedure, following the standard SEMR (**S**olve  $\rightarrow$  **E**stimate  $\rightarrow$  **M**ark  $\rightarrow$  **R**efine) process; see, for



**Figure 1:** Worst-case multi-objective error estimate  $\langle r(u^h), z^{h/2} \rangle$  for the Dirichlet–Poisson problem with solution (36) and objective set (38) versus  $\dim V_0^h$  for uniform finite-element spaces  $V_0^h$  with polynomial orders  $p \in \{1, 2, 3, 4\}$ . The solid lines indicate the actual errors  $\|u^h - u_{\text{osc}}\|_{L^2(\omega)}$ .

instance, [27, 9]. We consider the Dirichlet–Poisson problem (1) on an L-shaped domain  $\Omega = (-1, 1)^2 \setminus ([0, 1] \times (-1, 0])$ . The data  $f$  and  $g$  are selected such that  $u = u_{\text{sing}} + u_{\text{osc}}$  solves (1) with

$$u_{\text{sing}}(x, y) = \cos\left(\frac{\pi x}{2}\right) \cos\left(\frac{\pi y}{2}\right) (x^2 + y^2)^{1/3} \sin\left(\frac{2}{3} \arctan\left(\frac{y}{x}\right)\right) \quad (42)$$

and  $u_{\text{osc}}$  according to (36). Note that  $\gamma u = 0$  and, hence, the corresponding Dirichlet data  $g$  is homogeneous. The function  $u_{\text{sing}}$  in (42) exhibits a corner singularity at  $(0, 0)$ . In particular, it holds that  $u_{\text{sing}} \in H^s(\Omega)$  for  $s < 5/3$ ; see, for instance, [27]. It is well known that finite-element approximations on uniform meshes display suboptimal convergence rates, owing to the singularity in the solution. On uniform meshes, the error  $\|u^h - u_{\text{sing}}\|_{H^1(\Omega)}$  in the best approximation in  $V_0^h$  is only proportional to  $h^{2/3}$ , independent of the order of approximation [27]. Moreover, an Aubin–Nitsche duality argument conveys that  $\|u^h - u_{\text{sing}}\|_{L^2(\Omega)}$  decays only as  $h^{4/3}$ . The purpose of an adaptive finite-element method is to restore optimal convergence rates with respect to the dimension of the approximation space.

The objective set for the worst-case multi-objective error-estimation proce-

dure is again selected in accordance with (38) and, hence, the support function of  $\mathcal{O}$  corresponds to the  $\|\cdot\|_{L^2(\omega)}$ -norm of the error in the finite element approximation in the set  $\omega = (-3/4, -1/4)^2$ ; see Figure 2 for an illustration. The adaptive-refinement process based on the aforementioned error estimate thus endeavors to restore the optimal rate of convergence of  $\|u^h - u\|_{L^2(\omega)}$  with respect to  $\dim V_0^h$ . The applied SEMR process is illustrated in Figure 2. Given a mesh  $\mathcal{T}^h$ , we determine the finite-element approximation in the corresponding finite-element space,  $u^h \in V_0^h$ ; see panel (2,1) of Figure 2. We then construct the refined mesh,  $\mathcal{T}^{h/2}$ , by uniformly subdividing each element of  $\mathcal{T}^h$  into 4 elements, and determine the finite-element approximation  $u^{h/2} \in V_0^{h/2}$ ; see panel (1,2). Based on  $u^{h/2}$  and  $u^h$ , the error in the finite-element solution in  $V_0^h$  is estimated as  $u^{h/2} - u^h$  (panel (2,2)). The error estimate  $u^{h/2} - u^h$  serves to construct the approximate dual solution  $z^{h/2} \in V_0^{h/2}$  corresponding to the supporting functional of the objective set  $\mathcal{O}$  in (38), in accordance with (41) (panel (2,3)). Based on  $u^h$  and  $z^{h/2}$ , we determine the worst-case multi-objective error estimate  $\langle r(u^h), z^{h/2} \rangle$ . The error estimate is subsequently decomposed into local contributions, associated with the support of basis functions in  $V_0^{h/2}$ ; see panel (3,2). Let us note that instead of a traditional element-wise marking strategy, we apply the function-support marking strategy introduced in [23] (see also [35]). To elaborate on this strategy, let  $\{\psi_i\}_{i \in \mathcal{I}}$  with  $\mathcal{I} \subset \mathbb{N}$  denote the applied basis of  $V_0^{h/2}$  and let  $\Pi$  denote a suitable projection from  $V_0^{h/2}$  to  $V_0^h$ . In particular, we apply an  $L^2$ -projection for reasons of implementational convenience. The difference between the approximate dual solution and its projection onto  $V_0^h$  resides in  $V_0^{h/2}$  and can therefore be expanded as  $z^{h/2} - \Pi z^{h/2} = \sum \sigma_i \psi_i$ . Hence, we can decompose the DWR error estimate into fine-mesh basis-function contributions as:

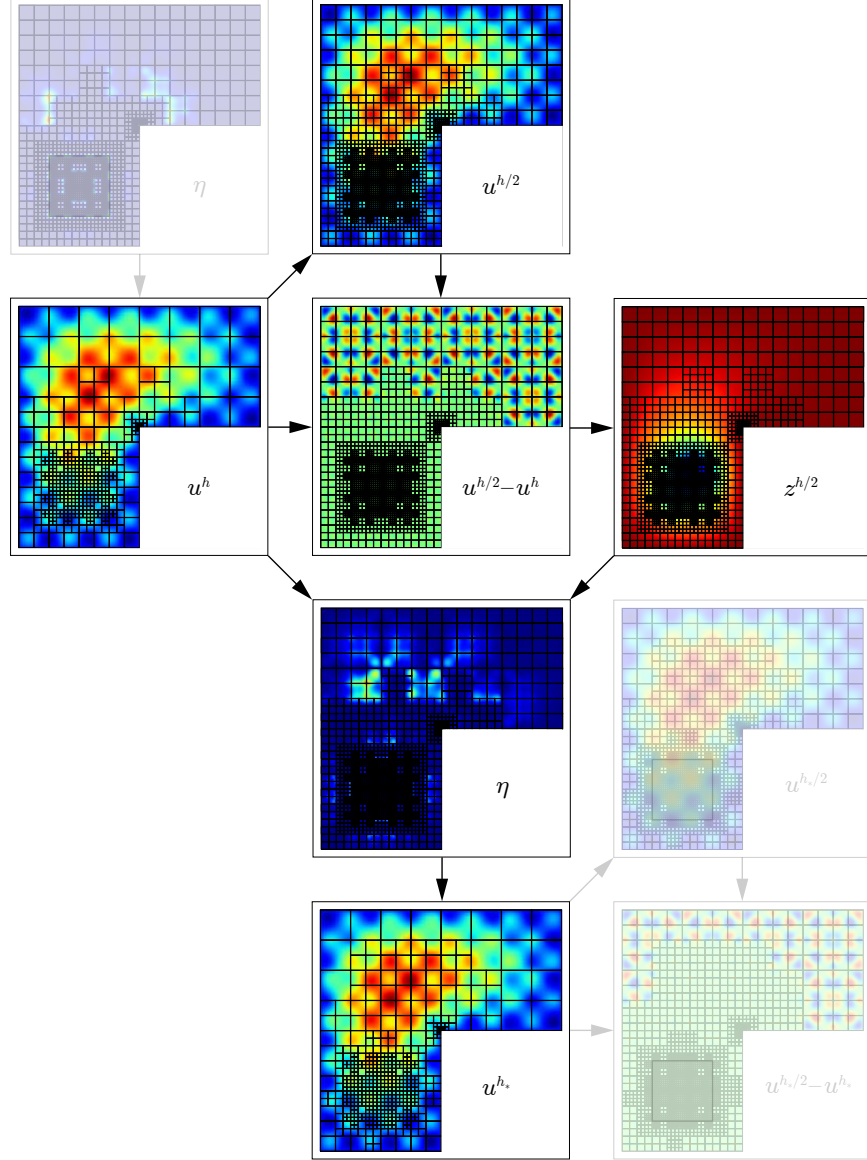
$$|\langle r(u^h), z^{h/2} - \Pi z^{h/2} \rangle| = \left| \sum_{i \in \mathcal{I}} \sigma_i \langle r(u^h), \psi_i \rangle \right| \leq \sum_{i \in \mathcal{I}} \eta_i \quad (43)$$

with  $\eta_i = |\sigma_i \langle r(u^h), \psi_i \rangle|$ . Based on the basis-function indicators,  $\{\eta_i\}$ , we mark basis functions according to a Dörfler-type [9] marking, i.e. we select a minimal set of indices  $\mathcal{A} \subset \mathcal{I}$  such that

$$\sum_{i \in \mathcal{A}} \eta_i \geq (1 - \zeta) \sum_{i \in \mathcal{I}} \eta_i \quad (44)$$

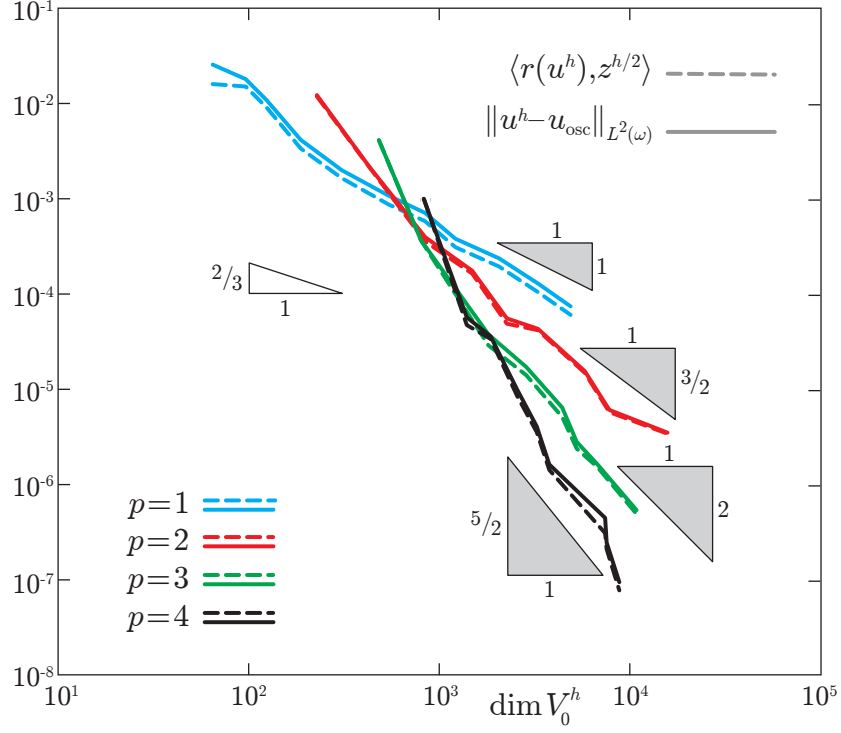
for some  $\zeta \in (0, 1)$ . In particular, we set  $\zeta = 1/2$ . Finally, we select a minimal set of coarse-grid elements,  $\mathcal{M}$ , such that the union of the supports of all marked basis functions,  $\cup_{i \in \mathcal{A}} \text{supp}(\psi_i)$ , is contained in the union of the selected elements,  $\cup_{K \in \mathcal{M}} K$ . These elements are subsequently partitioned to form a new mesh and to construct a corresponding new refined finite-element space; see panel (4,2).

Figure 3 plots the worst-case multi-objective error estimate  $\langle r(u^h), z^{h/2} \rangle$  and the error  $\|u^h - u\|_{L^2(\omega)}$  corresponding to the finite-element approximation  $u^h$  generated by the SEMR algorithm, versus the dimension of the adaptively refined finite-element space,  $\dim V_0^h$ , for finite-element approximations with polynomial orders  $p \in \{1, 2, 3, 4\}$ . The results convey that for all considered polynomial orders, the SEMR algorithm restores the optimal rate of convergence, i.e.,



**Figure 2:** Illustration of the worst-case multi-objective error-estimation process and the corresponding adaptive-refinement procedure. The square in each panel indicates the set  $\omega = (-3/4, -1/4)^2$  in which the  $L^2$ -norm of the error is to be minimized, in accordance with the objective set  $\mathcal{O}$  in (38).





**Figure 3:** Worst-case multi-objective error estimate  $\langle r(u^h), z^{h/2} \rangle$  and exact error  $\|u^h - u\|_{L^2(\omega)}$  versus  $\dim V_0^h$ , for sequences of adaptive finite-element approximations with polynomial orders  $p \in \{1, 2, 3, 4\}$  of the Dirichlet–Poisson problem on an L-shaped domain with solution  $u = u_{\text{osc}} + u_{\text{sing}}$ . The white triangle indicates the ( $p$ -independent) convergence rate corresponding to uniform mesh refinement.

the sequence of finite-element approximations generated by the SEMR algorithm exhibits a convergence rate proportional to  $(\dim V_0^h)^{-(p+1)/2}$ . It is noteworthy that the deviation between the actual error and the worst-case multi-objective error estimate is generally small.

#### 4.3. Worst-case multi-objective error estimation with data incompatibility

To illustrate the worst-case multi-objective error-estimation procedure with data incompatibility, we consider the unit square  $\Omega = (0, 1)^2$  and the Dirichlet–Neumann–Laplace problem:

$$-\nabla \cdot (\varepsilon \nabla u) = 0 \quad \text{in } \Omega \quad (45a)$$

$$u = g \quad \text{on } \Gamma_D \quad (45b)$$

$$\varepsilon \partial_n u = 0 \quad \text{on } \Gamma_N \quad (45c)$$

with  $\Gamma_D = ((0, 1] \times \{1\}) \cup (\{1\} \times (0, 1])$  and  $\Gamma_N = \partial\Omega \setminus \Gamma_D$ . The Dirichlet data  $g : \Gamma_D \rightarrow \mathbb{R}$  are given by:

$$g = \begin{cases} -\log((1-2x) + \nu 2x) & \text{if } (x, y) \in (0, 1/2] \times \{1\} \\ -\log((2x-1) + \nu(2-2x)) & \text{if } (x, y) \in (1/2, 1] \times \{1\} \\ \log((1-3x) + \nu 3x) & \text{if } (x, y) \in \{1\} \times (0, 1/3] \\ \log((3x-1)/2 + \nu 3(1-x)/2) & \text{if } (x, y) \in \{1\} \times (1/3, 1] \end{cases} \quad (46)$$

with  $\nu = 10^{-1}$ ; see Figure 4. The boundary data has been selected such that it exhibits nearly singular behavior at  $(x, y) \in \{1/2\} \times \{1\}$  and at  $(x, y) \in \{1\} \times \{1/3\}$ . The location of the latter point is such that it does not correspond to a vertex of the finite-element mesh for any finite refinement by uniform subdivision. We consider (45) with both a homogeneous coefficient  $\varepsilon = 1$  and a heterogeneous coefficient as depicted in 4.

Problem (45) can be conceived of as a Darcy-type problem, with  $u$  acting as pressure and  $-\varepsilon \nabla u$  the flux induced by the pressure gradient in a medium with isotropic permeability  $\varepsilon : \Omega \rightarrow \mathbb{R}_{>0}$ . In this setting, the Dirichlet condition (45b) imposes a prescribed pressure on  $\Gamma_D$  and the homogeneous Neumann condition (45c) corresponds to an impermeability condition on  $\Gamma_N$ . The heterogeneous permeability field is a smoothed version of a typical permeability field used in geostatistics in hydraulic diffusivity inversion. The permeability data is provided on a uniform mesh of  $628 \times 628$  points and is linearly interpolated between the data points to construct a continuous permeability field.

Denoting by  $H_{0,\Gamma_D}^1(\Omega)$  the subspace of  $H^1(\Omega)$  of functions that vanish on  $\Gamma_D$  in the trace sense, and by  $\ell_g$  a lift of  $g$  into  $H^1(\Omega)$  such that  $(\gamma \ell_g)|_{\Gamma_D} = g$ , the boundary value problem (45) can be condensed into the weak formulation: Determine  $u = u_0 + \ell_g$  with

$$u_0 \in H_{0,\Gamma_D}^1(\Omega) : \quad a_\varepsilon(u_0, v) = -a_\varepsilon(\ell_g, v) \quad \forall v \in H_{0,\Gamma_D}^1(\Omega) \quad (47)$$

and  $a_\varepsilon : H^1(\Omega) \times H^1(\Omega) \rightarrow \mathbb{R}$  according to:

$$a_\varepsilon(u, v) = \int_{\Omega} \varepsilon \nabla u \cdot \nabla v \quad (48)$$

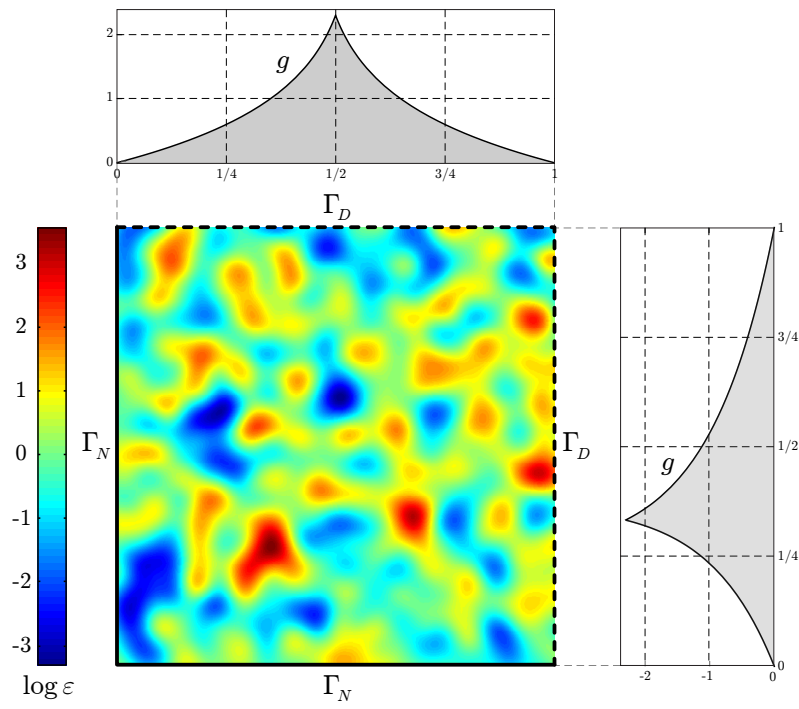
In conjunction with (47), we consider an objective set that is associated with the flux functional on a subset  $\omega \subseteq \Gamma_D$ :

$$\mathcal{O} = \left\{ j \in [H^1(\Omega)]^* : j(\cdot) = a_\varepsilon(\cdot, l_\lambda), \lambda \in H_{0,\partial\Omega \setminus \omega}^{1/2}(\partial\Omega), \|\lambda\|_{H^{1/2}(\partial\Omega)} \leq 1 \right\} \quad (49)$$

where  $H_{0,\partial\Omega \setminus \omega}^{1/2}(\partial\Omega)$  represents the subset of functions in  $H^{1/2}(\partial\Omega)$  that vanish on  $\partial\Omega \setminus \omega$ , and  $l_\lambda$  is the Moore–Penrose lift of  $\lambda$  with respect to the norm induced by  $a_\varepsilon$ :

$$l_\lambda = \arg \min \{ a_\varepsilon(v, v) : v \in H^1(\Omega), \gamma v = \lambda \} \quad (50)$$

Furthermore, in (49) we have introduced the norm  $\|\lambda\|_{H^{1/2}(\partial\Omega)}^2 = (\lambda, \lambda)_{H^{1/2}(\partial\Omega)}$  corresponding to the inner product  $(\varphi, \lambda)_{H^{1/2}(\partial\Omega)} = a_\varepsilon(l_\varphi, l_\lambda)$ .



**Figure 4:** Illustration of the setup of the third test case. Colors encode the logarithm of the heterogeneous permeability,  $\log \varepsilon$ .

The objective set (49) conforms to (34) with, in particular,  $T = H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega)$  and  $L : \lambda \mapsto l_\lambda$ . From (35) we then infer that the worst-case multi-objective error satisfies

$$\begin{aligned} & \sup \left\{ a_\varepsilon(u - u^h, l_\lambda) : \lambda \in H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega), \|\lambda\|_{H^{1/2}(\partial\Omega)} \leq 1 \right\} \\ &= \sup \left\{ a_\varepsilon(l_\varphi, l_\lambda) : \lambda \in H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega), \|\lambda\|_{H^{1/2}(\partial\Omega)} \leq 1 \right\} = \sqrt{a_\varepsilon(l_\varphi, l_\varphi)} \quad (51) \end{aligned}$$

with  $\varphi \in H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega)$  according to:

$$\varphi \in H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega) : \quad a_\varepsilon(l_\varphi, l_\lambda) = a_\varepsilon(u - u^h, l_\lambda) \quad \forall \lambda \in H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega) \quad (52)$$

To elucidate the relation between (51) and (35), we note that the left member of (52) coincides with the inner product  $(\varphi, \lambda)_{H^{1/2}(\partial\Omega)}$  and that the right member of (52) corresponds to the functional  $\hat{j}(\cdot) := a_\varepsilon(u - u^h, l_{(\cdot)}) \in [H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega)]^*$ . Equation (52) therefore constitutes a map  $\hat{j} \mapsto \phi(\hat{j}) = \varphi$ , corresponding to the canonical isometry:

$$\phi : [H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega)]^* \rightarrow H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega) \quad (53)$$

Furthermore, it holds that  $\|\phi(\hat{j})\|_{H^{1/2}(\partial\Omega)}^2 = (\varphi, \varphi)_{H^{1/2}(\partial\Omega)} = a_\varepsilon(l_\varphi, l_\varphi)$ .

In computations, it is impractical to extract  $\varphi$  directly from (52), on account of the implicit dependence of the inner product  $a_\varepsilon(l_{(\cdot)}, l_{(\cdot)})$  on the lift operator  $l_{(\cdot)}$ . To reformulate (52) into a tractable equivalent form, we note that the optimality conditions associated with (50) imply that

$$a_\varepsilon(v, l_\lambda) = 0 \quad \forall v \in H_0^1(\Omega) \quad (54)$$

By virtue of (54) and the symmetry of  $a_\varepsilon$ , Equation (52) implies

$$a_\varepsilon(l_\varphi, l_\lambda + v) = a_\varepsilon(u - u^h + q, l_\lambda + v) \quad \forall v \in H_0^1(\Omega) \quad (55)$$

provided that  $q \in H_0^1(\Omega)$  satisfies

$$q \in H_0^1(\Omega) : \quad a_\varepsilon(q, v) = -a_\varepsilon(u - u^h, v) \quad \forall v \in H_0^1(\Omega) \quad (56)$$

Because  $(\lambda, v) \mapsto l_\lambda + v$  provides a bijection between  $H_{0,\partial\Omega\backslash\omega}^{1/2}(\partial\Omega) \times H_0^1(\Omega)$  and  $H_{0,\partial\Omega\backslash\omega}^1(\Omega)$ , Equation (55) implies that  $l_\varphi$  is the unique element of  $H_{0,\partial\Omega\backslash\omega}^1(\Omega)$  in compliance with:

$$l_\varphi \in H_{0,\partial\Omega\backslash\omega}^1(\Omega) : \quad a_\varepsilon(l_\varphi, v) = a_\varepsilon(u - u^h + q, v) \quad \forall v \in H_{0,\partial\Omega\backslash\omega}^1(\Omega) \quad (57)$$

Problem (57) is in canonical form. Hence,  $l_\varphi$  can be conveniently extracted from (57) and  $\varphi$  can in turn be obtained directly from the identity  $\varphi = \gamma(l_\varphi)$ .

The exact solution  $u$  is generally not available. Also, Eqs. (56)-(57) cannot generally be solved. In the numerical computations, we therefore have to

replace  $u$  and  $q$  by computable approximations. We opt to replace  $u$  by an approximation  $u^{h/2}$  obtained in the refined finite-element space  $V^{h/2}$ . In addition, we replace  $q$  and  $l_\varphi$  by  $q^{h/2}$  and  $l_\varphi^{h/2}$ , respectively, according to:

$$q^{h/2} \in V_0^{h/2} : \quad a_\varepsilon(q^{h/2}, v^{h/2}) = -a_\varepsilon(u^{h/2} - u^h, v^{h/2}) \quad \forall v^{h/2} \in V_0^{h/2} \quad (58)$$

$$l_\varphi^{h/2} \in V_{0, \partial\Omega \setminus \omega}^{h/2} : \quad a_\varepsilon(l_\varphi^{h/2}, v^{h/2}) = a_\varepsilon(u^{h/2} - u^h + q^{h/2}, v^{h/2}) \quad \forall v^{h/2} \in V_{0, \partial\Omega \setminus \omega}^{h/2} \quad (59)$$

with  $V_{0, \partial\Omega \setminus \omega}^{h/2} := V^{h/2} \cap H_{0, \partial\Omega \setminus \omega}^1(\Omega)$ .

If the worst-case multi-objective error estimate is to be applied in an adaptive-refinement process, then a decomposition of the error into basis-function contributions must be introduced, cf. Equation (43). Denoting by  $\{\psi_i\}$  a basis of  $V_{0, \partial\Omega \setminus \omega}^{h/2}$ , there exist coefficients  $\{\sigma_i\}$  such that:

$$\frac{l_\varphi^{h/2}}{\|l_\varphi^{h/2}\|_{H^{1/2}(\partial\Omega)}} = \sum \sigma_i \psi_i \quad (60)$$

Hence, the worst-case multi-objective error estimate can be decomposed and bounded as:

$$\frac{|a_\varepsilon(u^{h/2} - u^h, l_\varphi^{h/2})|}{\|l_\varphi^{h/2}\|_{H^{1/2}(\partial\Omega)}} = \left| \sum_{i \in \mathcal{I}} \sigma_i a_\varepsilon(u^{h/2} - u^h, \psi_i) \right| \leq \sum_{i \in \mathcal{I}} \eta_i \quad (61)$$

with  $\eta_i = |\sigma_i a_\varepsilon(u^{h/2} - u^h, \psi_i)|$ . From (58) and (59) it however follows that

$$a_\varepsilon(u^{h/2} - u^h, l_\varphi^{h/2}) = a_\varepsilon(u^{h/2} - u^h + q^{h/2}, l_\varphi^{h/2}) = a_\varepsilon(l_\varphi^{h/2}, l_\varphi^{h/2}) \quad (62)$$

The second and third expressions in (62) provide equivalent error estimates, and can alternatively serve to construct error bounds and error indicators analogous to (61). It is important to note, however, that although the error estimates in (62) are equivalent, the corresponding error bounds are generally not. From (59) one can infer that the error bounds derived from the second and third expressions in (62) coincide. However, these will generally deviate from the error bound derived from the first expression in (62).

To assess the accuracy of the worst-case multi-objective error estimates in (62) and the tightness of the corresponding error bounds, we consider finite-element approximations of (47) and the worst-case multi-objective error estimates and bounds:

$$\begin{aligned} \text{est}_1 &= \frac{|a_\varepsilon(u^{h/2} - u^h, l_\varphi^{h/2})|}{\|l_\varphi^{h/2}\|_{H^{1/2}(\partial\Omega)}} & \text{bnd}_1 &= \sum_{i \in \mathcal{I}} |\sigma_i a_\varepsilon(u^{h/2} - u^h, \psi_i)| \\ \text{est}_2 &= \frac{|a_\varepsilon(l_\varphi^{h/2}, l_\varphi^{h/2})|}{\|l_\varphi^{h/2}\|_{H^{1/2}(\partial\Omega)}} & \text{bnd}_2 &= \sum_{i \in \mathcal{I}} |\sigma_i a_\varepsilon(l_\varphi^{h/2}, \psi_i)| \end{aligned} \quad (63)$$

for  $\omega = \Gamma_D$ , i.e. we regard estimates of the worst-case error in the flux functional along the entire Dirichlet boundary. Figure 5 plots  $\text{est}_{1,2}$  and  $\text{bnd}_{1,2}$  according to (63) versus the dimension of the finite-element approximation space,  $\dim V_{0,\Gamma_D}^h$ , for standard finite-element approximations with polynomial degrees  $p \in \{1, 2, 3, 4\}$  on a sequence of uniform meshes with mesh widths  $h \in \{2^{-2}, 2^{-3}, \dots, 2^{-7}\}$ , and for the homogeneous permeability  $\varepsilon = 1$  (*left*) and the heterogeneous permeability in Figure 4 (*right*). In addition, Figure 5 plots a reference error estimate according to

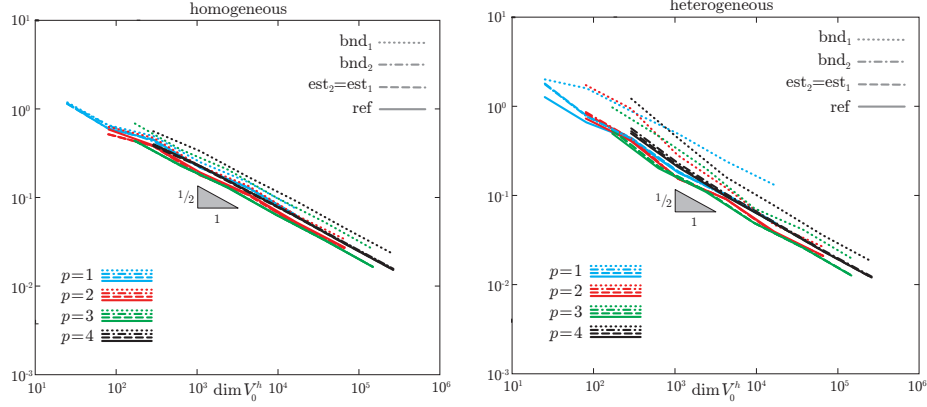
$$\text{ref} = \frac{|a_\varepsilon(u^{h_{\text{ref}}} - u^h, l_\varphi^{h_{\text{ref}}})|}{\|l_\varphi^{h_{\text{ref}}}\|_{H^{1/2}(\partial\Omega)}} \quad (64)$$

with  $h_{\text{ref}} = 2^{-8}$ . Comparison of the solid and dashed curves in Figure 5 indicates that the error estimates  $\text{err}_{1,2}$  generally provide accurate estimates of the worst-case multi-objective error, even on coarse meshes. Only for the heterogeneous case,  $p = 1$  and coarse meshes ( $h \in \{2^{-2}, 2^{-3}\}$ ) there is a noticeable deviation between  $\text{err}_{1,2}$  and the reference error estimate. Figure 5 moreover reveals a significant difference between  $\text{bnd}_1$  and  $\text{bnd}_2$ , despite the fact that these bounds derive from equivalent error estimates. While  $\text{bnd}_2$  is tight and the deviation between the estimates  $\text{err}_{1,2}$  and the bound  $\text{bnd}_2$  is generally not discernible, the bound  $\text{bnd}_1$  typically deviates from  $\text{err}_{1,2}$  by a factor of 2 or more. The deviation between  $\text{bnd}_1$  and  $\text{err}_{1,2}$  is particularly manifest for the heterogeneous-permeability case. One may also observe from Figure 5 that both in the homogeneous and heterogeneous case, the error decays only as  $(\dim V_{0,\Gamma_D}^h)^{1/2}$ , independent of the order of approximation. This suboptimal convergence behavior is attributable to the fact that the near-singularities in the Dirichlet data are not resolved on the considered meshes.

#### 4.4. Worst-case multi-objective error estimation and adaptivity with data incompatibility

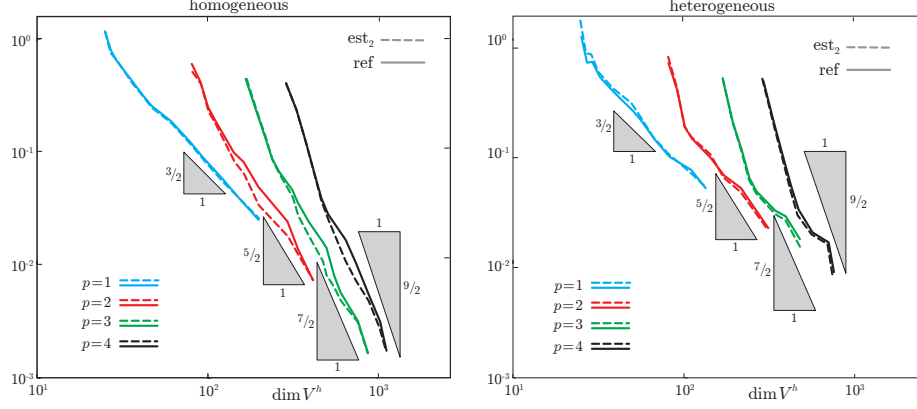
In this section we consider worst-case multi-objective error estimation and adaptivity for weak formulation (47) in conjunction with objective set (49). The adaptive-refinement procedure based on the worst-case multi-objective error estimate associated with (49) essentially aims to construct a finite-element space that yields an optimal approximation of the flux functional  $-\varepsilon \partial_n u$  on  $\omega = \Gamma_D$ . We again consider the bilinear form (48) with both a homogeneous coefficient  $\varepsilon = 1$  and a heterogeneous coefficient according to Figure 4. Recalling that  $\text{bnd}_2$  in (63) generally provides a tighter bound of the error estimate than  $\text{bnd}_1$ , we base the marking strategy in the SEMR procedure on the error indicators  $\eta_i = |\sigma_i a_\varepsilon(l_\varphi^{h/2}, \psi_i)|$ , i.e. the summands in  $\text{bnd}_2$ . The marking and refinement operations are otherwise identical to those described in Section 4.2. The initial mesh for the adaptive computations is composed of  $4 \times 4$  elements.

Figure 6 displays the worst-case multi-objective error estimate  $\text{est}_2$  according to (63) corresponding to the finite-element approximation  $u^h$  generated by the SEMR algorithm, versus the dimension of the adaptively refined finite-element



**Figure 5:** Worst-case multi-objective error estimates  $\text{est}_1$  and  $\text{est}_2$  (coincident) for test case 3 with homogeneous coefficients (*left*) and heterogeneous coefficient (*right*), and upper bounds  $\text{bnd}_1$  and  $\text{bnd}_2$  according to (63) versus the number of degrees of freedom for finite-element spaces with polynomial orders  $p \in \{1, 2, 3, 4\}$  on uniform meshes. The solid lines indicate the reference error estimates according to (64).

space for finite-element approximations with polynomial orders  $p \in \{1, 2, 3, 4\}$ . Results for the homogeneous coefficient  $\varepsilon = 1$  and the heterogeneous coefficient according to Figure 4 are presented in the left and right panels of Figure 6, respectively. In addition to the error estimate  $\text{est}_2$ , Figure 6 displays a reference error estimate conforming to (64) with  $V^{h_{\text{ref}}}$  the finite-element space that is obtained by uniform bisection of all elements in the final mesh constructed by the adaptive algorithm. It is noteworthy that the deviation between the error estimate and the reference error estimate is generally small. The left panel of Figure 6 indicates that in the homogeneous case, the adaptive-refinement procedure yields a convergence rate proportional to  $(\dim V^h)^{-(p+1/2)}$ . A similar convergence rate appears to hold for the heterogeneous case, although the results in the right panel of Figure 6 are less conclusive. It is to be noted, however, that for the heterogeneous case the refinement procedure reaches the resolution of the permeability data ( $628 \times 628$ ) after 7 levels of refinement, which affects the asymptotic convergence rate. We conjecture that the convergence rate  $(\dim V^h)^{-(p+1/2)}$  corresponds to optimal convergence in the  $H^{1/2}$ -norm in 1 dimension, but such approximability results in fractional-order Sobolev spaces have to our knowledge only been established for piecewise-linear approximations [8]. It is remarkable that the convergence rate achieved by the adaptive algorithm appears to pertain to approximation of a 1-dimensional object. This is however consistent with the fact that the worst-case multi-objective error corresponds to  $s(\mathcal{O}, u - u^h) = \|\varphi\|_{H^{1/2}(\partial\Omega)}$  with  $\varphi \in H_{0,\partial\Omega \setminus \omega}^{1/2}(\partial\Omega)$ ; see (51) and (52). It is therefore plausible that (for each  $p$ ) the adaptive algorithm generates a sequence of adaptive finite-element approximation spaces,  $\{V^h\}$ , such that the



**Figure 6:** Worst-case multi-objective error estimate  $\text{est}_2$  and reference error estimate for test case 3 with homogeneous coefficients (*left*) and heterogeneous coefficient (*right*), versus  $\dim V^h$  for sequences of adaptive finite-element approximations with polynomial orders  $p \in \{1, 2, 3, 4\}$ .

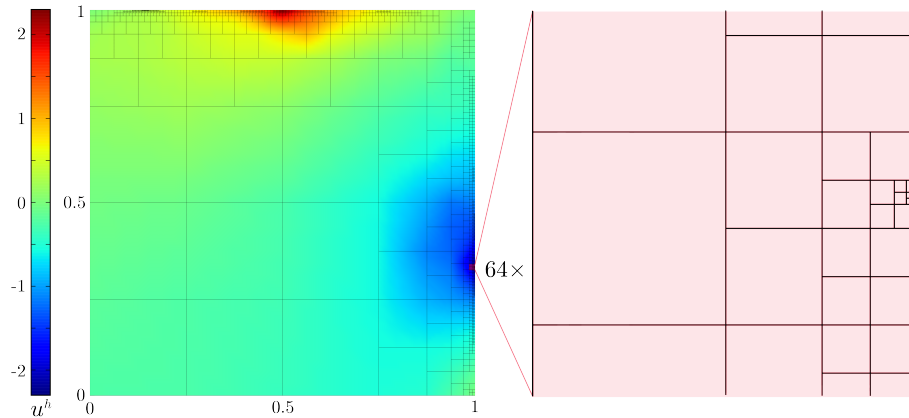
worst-case multi-objective error of the Galerkin approximations  $u^h \in V^h$  decays as  $s(\mathcal{O}, u - u^h) = \|\varphi\|_{H^{1/2}(\partial\Omega)} \propto (\dim V^h)^{-(p+1/2)}$  as  $\dim V^h \rightarrow \infty$ . A detailed analysis of this convergence behavior is beyond the scope of this work.

Figure 7 presents the finite-element mesh that is obtained after 16 iterations of the SEMR process for the test case with a heterogeneous coefficient, for a finite-element approximation of order  $p = 1$ . The red square in Figure 7 presents a magnification ( $64\times$ ) of the mesh near the nearly-singular point  $(x, y) = (1, 1/3)$ . One can observe that the mesh is refined towards the part of the boundary corresponding to  $\omega = \Gamma_D \subset \partial\Omega$  which constitutes the support of the functional  $-\varepsilon \partial_n u$  according to the objective set (49). Moreover, the adaptive refinement is most concentrates near the nearly-singular points and, in particular, near the irrational point  $(x, y) = (1, 1/3)$ . Comparing the mesh in Figure 7 with the value of the heterogeneous coefficient  $\varepsilon$  in Figure 4 on page 19, one can notice that the adaptive mesh is generally finer in regions where the coefficient (permeability) is relatively large. Let us also allude to the refinement near the bottom right corner,  $(x, y) = (1, 0)$ . It appears that a weak singularity occurs at this point due the transition between the Dirichlet boundary condition and the Neumann boundary condition.

## 5. Conclusion

In this work we introduced a new computational methodology for determining a-posteriori worst-case multi-objective error estimates for finite-element approximations. The methodology applies to both standard finite-element approximation errors and data-incompatibility errors due to incompatibility of





**Figure 7:** Finite-element mesh for test case 3 with heterogeneous coefficients for approximation order  $p = 1$ , after 16 iterations of the SEMR process. The red square presents a magnification ( $64\times$ ) of the mesh near the nearly-singular point  $(x, y) = (1, 1/3)$ .

boundary data with the trace of the finite-element space. As opposed to goal-oriented approaches, which consider only a single objective functional, the presented methodology applies to general closed convex subsets of the dual space. The worst-case multi-objective error coincides with the support function of the considered objective set at the finite-element approximation error. The error estimate presented in this work adopts a standard dual-weighted-residual form, in which the dual solution corresponds to an approximation of the supporting functional of the objective set at the approximation error. The error estimate can direct an adaptive-refinement procedure in a similar manner as in conventional goal-oriented approaches, rendering a multi-objective adaptive strategy.

To illustrate the properties of the worst-case multi-objective error-estimation technique and its application in adaptive refinement procedures, we presented numerical results for two Dirichlet–Poisson test cases with compatible boundary data and one Dirichlet–Neumann–Laplace test case with incompatible boundary data. In the numerical experiments, we considered an approximation of the supporting functional based on the finite-element approximation and a finite-element approximation on a mesh refined by uniform bisection. We generally observed very good agreement between the worst-case multi-objective error estimate thus obtained and the actual worst-case multi-objective error, even on coarse meshes and at low orders of approximation.

For the test case with incompatible boundary data, we derived two distinct but equivalent error estimates. We showed that in contrast to the equivalence of the error estimates, the error bounds obtained from these estimates are generally not equivalent. While one error bound was observed to be tight, the other displayed a significant deviation from the underlying error estimate.

For the considered test cases, application of the worst-case multi-objective error estimate in an adaptive refinement procedure resulted in optimal convergence rates. For the Dirichlet–Neumann–Laplace test case with data incompatibility, the adaptive algorithm yields a form of super-convergence, in that the obtained convergence rate corresponds to an optimal convergence rate for a function on a manifold of co-dimension 1.

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